CLAIMS

1. A Voigt function approximation calculating method used for line-by-line calculations, said method comprising:

(1) a step of dividing a domain of a Voigt function into a first range around the peak of the Voigt function and a skirt portion not contained in the first range, replacing the first range with a cubic function, calculating the values and derivatives of said cubic function and the Voigt function in the skirt portion for each of first predetermined intervals, and connecting said cubic function and said Voigt function at points of connection thereof using the values and derivatives of both functions;

(2) a step of adding together the results of step (1) for a plurality of absorption lines;

(3) a step of calculating the function values and derivatives for the results of step (2) by interpolation over intervals smaller than said first predetermined intervals;

(4) a step of dividing said first range into a second range near the peak and a skirt portion not contained in the second range, replacing said second range of a "function representing the difference between the Voigt function and said cubic function" with a cubic function, and calculating values and derivatives of said cubic function and said "function representing the difference between the Voigt function and said cubic function" in the skirt portion for each of second predetermined intervals;

(5) a step of connecting said cubic function and said "function representing the difference between the Voigt function and said cubic function" at points of connection thereof using the values and derivatives of both functions;

(6) a step of adding the results of steps (4) and (5) to the results of step (3) for a plurality of absorption lines;

(7) a step of calculating the function values and derivatives for the results of step (6)

by interpolation over intervals smaller than said second predetermined intervals; and

(8) a step of adding the values of the "function representing the difference between the Voigt function and said cubic function" to the results of step (7) for a plurality of absorption lines in said second range.

2. A method in accordance with claim 1, wherein (9) a step of calculating function values and derivative values by interpolation is repeated while narrowing the intervals until they become intervals of a minimum unit.

3. A method in accordance with claim 1, wherein said steps (4) through (7) are repeated one or more times until the third predetermined interval is obtained.

4. A method in accordance with claim 1, wherein said predetermined intervals are determined by using the following equation.

The first predetermined interval for the widest sub-function is $j^{kmax}dv$. Here, j is a single-digit natural number, dv is the increment in wave number, and $kmax$ is the largest natural number satisfying the relationship $j^{kmax+2}pdv \leq Vmax$. However, $Vmax$ represents the maximum calculation range from the center of the absorption line, and p is a natural number for controlling the calculation precision

5. A method in accordance with claim 3, wherein said predetermined intervals are determined using the following equation.

The most specific third predetermined interval is $j^{kmin}dv$. Here, j is a single-digit natural number, dv is the increment of the wave number, and $kmin$ is the maximum non-negative decimal fraction satisfying the relationship $j^{kmin}pdv \leq \alpha$ (α being approximately $\gamma/4$). However, γ is an approximate value of the full-width at half-max of the absorption line, and p is a natural number for controlling the calculation precision.

6. A method in accordance with claim 1, wherein said second predetermined intervals are determined by using the following equation.

For the sub-function with the ($k - kmin + 1$)-th smallest width, the predetermined interval is $j^k dv$. Here, j is a single-digit natural number, dv is the increase in wave number and k is such that $kmin \le k < kmax$.

7. A method in accordance with any one of claims 1-3, wherein said interpolation is calculated with j set to 4, using the function values y_0, y_1 and function derivative values y_0', y_1' at x_0, x_1 in the interpolation interval (x_0, x_1), with the below-given Equation (1) as a function value interpolation equation, Equation (2) as a function derivative value interpolation equation and ε as a non-negative decimal fraction.

$$\begin{pmatrix} y_a \\ y_b \\ y_c \end{pmatrix} = \frac{1}{64}\begin{pmatrix} 54-6\varepsilon & 10+6\varepsilon & 9(1-\varepsilon) & -3(1-\varepsilon) \\ 32 & 32 & 8(1-\varepsilon) & -8(1-\varepsilon) \\ 10+6\varepsilon & 54-6\varepsilon & 3(1-\varepsilon) & -9(1-\varepsilon) \end{pmatrix}\begin{pmatrix} y_0 \\ y_1 \\ (x_1-x_0)y_0' \\ (x_1-x_0)y_1' \end{pmatrix} \qquad (1)$$

$$\begin{pmatrix} y_a' \\ y_b' \\ y_c' \end{pmatrix} = \frac{1}{16(x_1-x_0)}\begin{pmatrix} -18+2\varepsilon & 18-2\varepsilon & 3(1-\varepsilon) & -5(1-\varepsilon) \\ -24+8\varepsilon & 24-8\varepsilon & -4(1-\varepsilon) & -4(1-\varepsilon) \\ -18+2\varepsilon & 18-2\varepsilon & -5(1-\varepsilon) & 3(1-\varepsilon) \end{pmatrix}\begin{pmatrix} y_0 \\ y_1 \\ (x_1-x_0)y_0' \\ (x_1-x_0)y_1' \end{pmatrix} \qquad (2)$$

8. A method in accordance with any one of claims 1-3, wherein said interpolation is calculated with j set to 5, using the function values y_0, y_1 and function derivative values y_0', y_1' at x_0, x_1 in the interpolation interval (x_0, x_1), with the below-given Equation (3) as a function value interpolation equation, Equation (4) as a function derivative value interpolation equation and ε as a non-negative decimal fraction.

$$\begin{pmatrix} y_a \\ y_b \\ y_c \\ y_d \end{pmatrix} = \frac{1}{125} \begin{pmatrix} 112-12\varepsilon & 13+12\varepsilon & 16(1-\varepsilon) & -4(1-\varepsilon) \\ 81-6\varepsilon & 44+6\varepsilon & 18(1-\varepsilon) & -12(1-\varepsilon) \\ 44+6\varepsilon & 81-6\varepsilon & 12(1-\varepsilon) & -18(1-\varepsilon) \\ 13+12\varepsilon & 112-12\varepsilon & 4(1-\varepsilon) & -16(1-\varepsilon) \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ (x_1-x_0)y_0' \\ (x_1-x_0)y_1' \end{pmatrix} \tag{3}$$

$$\begin{pmatrix} y_a' \\ y_b' \\ y_c' \\ y_d' \end{pmatrix} = \frac{1}{25(x_1-x_0)} \begin{pmatrix} -24-\varepsilon & 24+\varepsilon & 8(1-\varepsilon) & -7(1-\varepsilon) \\ -36+11\varepsilon & 36-11\varepsilon & -3(1-\varepsilon) & -8(1-\varepsilon) \\ -36+11\varepsilon & 36-11\varepsilon & -8(1-\varepsilon) & -3(1-\varepsilon) \\ -24-\varepsilon & 24+\varepsilon & -7(1-\varepsilon) & 8(1-\varepsilon) \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ (x_1-x_0)y_0' \\ (x_1-x_0)y_1' \end{pmatrix} \tag{4}$$

9. A method in accordance with any one of claims 1-8, for achieving high speeds, when assuming the Voigt function to be $K(x, y)$ and the difference from the Voigt profile of the absorption line to be $K(x, y) + f(x)$, replacing

$$K(x,y)$$

with:

$$\widetilde{K}(x,y) = AK(x,y) + Bf(x)$$

and

$$\frac{\partial K(x,y)}{\partial x}$$

with

$$\frac{\partial \widetilde{K}(x,y)}{\partial x} = A\frac{\partial K(x,y)}{\partial x} + B\frac{\partial f(x)}{\partial x}$$

10. A method in accordance with any one of claims 1-8, for achieving high speeds, when assuming the Voigt function to be $K(x, y)$ and the difference from the Voigt profile of the absorption line to be $K(x, y)f(x)$, replacing

$$K(x,y)$$

with:

$$\tilde{K}(x,y) = K(x,y)f(x)$$

and

$$\frac{\partial K(x,y)}{\partial x}$$

with

$$\frac{\partial \tilde{K}(x,y)}{\partial x} = \frac{\partial K(x,y)}{\partial x} f(x) + K(x,y)\frac{\partial f(x)}{\partial x}$$

11. A method in accordance with any one of claims 1-10, for achieving high speeds in a sub-Lorentzian correction, by using

$$\tilde{K}(x,y) = K(x,y)A\exp(-B|x|)$$

and

$$\frac{\partial \tilde{K}(x,y)}{\partial x} = \frac{\partial K(x,y)}{\partial x} A\exp(-B|x|) + K(x,y)[-\operatorname{sgn}(x)AB\exp(-B|x|)]$$

12. A method in accordance with any one of claims 1-10, for achieving high speeds in line-mixing correction, by replacing

$$K(x,y)$$

with:

$$\tilde{K}(x,y) = AK(x,y) + BL(x,y)$$

and

$$\frac{\partial K(x,y)}{\partial x}$$

with

$$\frac{\partial \tilde{K}(x,y)}{\partial x} = -2\left[(Ax+By)K(x,y) - (Ay-Bx)L(x,y) - \frac{B}{\sqrt{\pi}}\right]$$

Here, $L(x, y)$ is the imaginary component of the function $w(z)$ (the real part is the Voigt

function), where complex number $z = x + iy$, defined by the following equation.

$$w(z) = \frac{i}{\pi}\int_{-\infty}^{\infty}\frac{\exp(-t^2)}{z-t}dt = \exp(-z^2)erfc(-iz) = K(x,y) + iL(x,y)$$

($erfc(z)$ is a complex complementary error function).

13. A Voigt function approximation calculating program used for line-by-line calculations, said program performing:

(1) a step of dividing a domain of a Voigt function into a first range around the peak of the Voigt function and a skirt portion not contained in the first range, replacing the first range with a cubic function, calculating the values and derivatives of said cubic function and the Voigt function in the skirt portion for each of a first predetermined intervals, and connecting said cubic function and said Voigt function at points of connection thereof using the values and derivatives of both functions;

(2) a step of adding together the results of step (1) for a plurality of absorption lines;

(3) a step of calculating the function values and derivatives for the results of step (2) by interpolation over intervals smaller than said first predetermined intervals;

(4) a step of dividing said first range into a second range near the peak and a skirt portion not contained in the second range, replacing said second range of a "function representing the difference between the Voigt function and said cubic function" with a cubic function, and calculating values and derivatives of said cubic function and said "function representing the difference between the Voigt function and said cubic function" in the skirt portion for each of second predetermined intervals;

(5) a step of connecting said cubic function and said "function representing the difference between the Voigt function and said cubic function" at points of connection thereof using the values and derivatives of both functions;

(6) a step of adding the results of steps (4) and (5) to the results of step (3) for a

plurality of absorption lines;

(7) a step of calculating the function values and derivatives for the results of step (6) by interpolation over intervals smaller than said second predetermined intervals; and

(8) a step of adding the values of the "function representing the difference between the Voigt function and said cubic function" to the results of step (7) for a plurality of absorption lines in said second range.

14. A program in accordance with claim 13, wherein a step of calculating function values and derivative values by interpolation is repeated while narrowing the intervals until they become intervals of a minimum unit.

15. A program in accordance with claim 13, wherein said steps (4) through (7) are repeated one or more times until the third predetermined interval is obtained.